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Toward Modeling Limited Plasticity in Ceramic Materials

by Michael Grinfeld, Scott E. Schoenfeld, and Tim W. Wright

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14. ABSTRACT

The characteristic features of many armor-related ceramic materials are the anisotropy on the micro-scale level and the very limited, though non-vanishing, plasticity due to limited number of the planes for plastic slip. This work in progress is targeted toward revising phenomenological models of such materials with limited number of slip planes. In order to emphasize the key ideas of our approach, we illustrate the approach using the simplest possible model, the so-called "deck-of-cards" model.

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1. Introduction: Some Earlier Efforts

The theory of plasticity was originally formulated on the basis of purely phenomenological approach. The monograph of Hill (*1*) reviews the contributions of Tresca, von Mises, Drucker, Timoshenko, Illyushin, and many other mechanists and mathematicians who used this approach. The macroscopic hysteresis, i.e., of the dependence of the "strain-stress" relationships upon the history of loading, was the central physical phenomenon studied during this period. When using the purely macroscopic and phenomenological methods, the microscopic physical mechanisms of the hysteresis remain unexplained. Such a direct analysis of the macroscopic experiment has its strong features. Among them, for instance, the absence of any unnecessary ad hoc hypothesis, the reduced theoretical ambiguities in the models, and the conceptual simplicity in interpretation of experimental data and theoretical results. On the other hand, all the results of the earlier plasticity theory were about statics, dynamics, and optimization of *structures*—not about the physical properties of *materials*.

Taylor (*2*) and his contemporaries made a major breakthrough in the physics of plasticity by introducing a theoretical concept of dislocation as the micro-mechanism of plasticity and showing its practical fruitfulness. Later on, the experimental observations of the dislocations have been reported in many publications (see a detailed review by Hirth [*3*]). The success and impact of this concept is too multifaceted to be discussed here. On the theoretical side, however, there are some serious technical drawbacks in dealing with dislocations, which include, among others, the necessity of dealing with singular elastic fields in the vicinity of dislocations cores and much bigger overall difficulties for the theoretical analysis (using methods matching asymptotic expansions, methods of homogenizations, essentially more difficult boundary value problems, etc.).

The acceptance of the dislocation-based mechanism of plasticity entailed many different attempts to describe the behavior of ensembles of dislocations. Naturally, there were even attempts to derive the classical equations of macroscopic plasticity by means of homogenization of the microscopic ensembles of dislocations. All these efforts, unfortunately, were not successful. One of the Russian plasticity authorities—Yuri Rabotnov—even claimed (*4*) that he does not believe in the possibility of deriving phenomenological equations of macroscopic plasticity by means of convincing homogenization of any microscopic models.

We strongly believe, however, that, at present, the essential progress in this direction can be achieved. Our belief is based on the progress, reached during last decades in thermodynamics of heterogeneous systems, from one hand, and in the development of rigorous mathematical theories of homogenization (*5*, *6*). The central theoretical notion of the mathematical theory of

homogenization is the elementary cell of the structure. The main technical tools of this theory are the so-called G-convergence and the asymptotic method of the two-scale asymptotic expansions (*7*).

When homogenizing the periodic microstructures of dislocations, the elementary cell is just a parallelepiped of periodicity containing a single dislocation. This sort of microstructure is not easy to handle in a rigorous way because, currently, the descriptions of the individual dislocations, on their own, are far of to be rigorous enough. There are more chances of achieving success using the microstructures proposed by Batdorf and Budiansky (*8*). Instead of using a micro-model of dislocation, they used as the building brick for their theory the concept of elementary slip within an elementary mono-crystallites. Their approach was further developed and reviewed in the summarizing monograph (*9*). Strategically, we keep in mind this very micro-model of plasticity in our efforts to suggest a macroscopic theory of limited plasticity.

2. Typical Microstructures

Practically, in any real polycrystalline material, the system of monocrystalline grains is a chaotic ensemble with stochastic distributions of sizes, shapes, crystallographic orientations, etc., similar to those in figure 1.

Figure 1. Microstructure of polycrystalline substance.

There is considerable progress in the theoretical problem of homogenization of stochastic microstructures. But it is much more complex than homogenization of periodic microstructures (*5*–*7*). This difficulty is not purely technical: in fact, it has purely physical roots. The stochastic microstructures are characterized by much more complex physical phenomena than, say, periodic microstructures. Nonetheless, there are also many physical and mathematical similarities in the behavior and in the mathematical analysis of the stochastic and periodic microstructures. Basically, theoretical homogenization of periodic microstructures is much

simpler and transparent. Theorists dealing with sintering of ceramics (*10*) traditionally concentrate first on heterogeneous system with periodic distributions of monocrystalline grains, such as a hexagonal system shown in figure 2a.

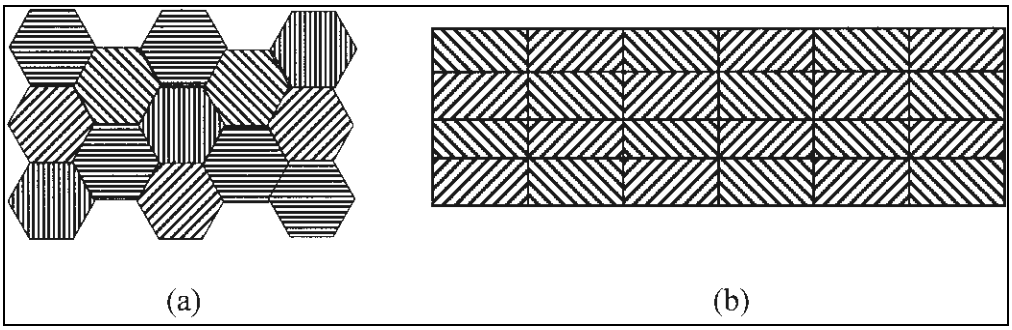

Figure 2. Models of ensembles of periodically distributed crystallites with stochastically (a) and periodically (b) distributed orientations of single slip systems.

Each mono-crystalline grain behaves as an elasto-plastic solid. The elastic behavior is nothing more than the displacements of particles in which atomic order of particles does not change. The inelastic behavior, by definition, includes processes involving essential changes on the atomic order. The simplest model of inelasticity is associated with slippage along preferably oriented plane. A plastic slip system is a set of parallel atomic planes of a special crystallographic orientation. Each of those planes split the crystal into two parts, and the two parts can easily slide with respect to the other as a whole (see figure 3). In the process of sliding, the atoms adjacent to the corresponding slip plane, change their neighbors on the opposite side of plane. Although the shape of the individual mono-crystals changes considerably, the mono-crystalline character of the substance remains preserved.

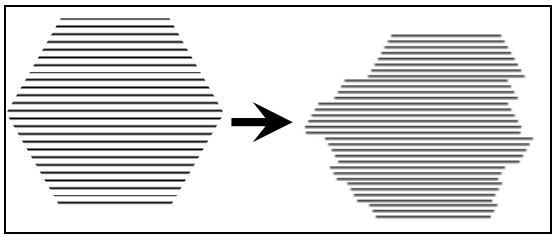

Figure 3. The system of plastic slip within crystalline substance.

A highly plastic crystalline substance possesses many different slip systems, supplying the crystal with many degrees of freedom for changing its shape when adjusting to external loading. The more slip families exist the more pronounced is the plastic behavior. The crystal with a single slip system shows very limited plasticity—this makes such a model particularly promising for modeling polycrystalline ceramics.

For rigorous theoretical analysis, however, further simplifications of the model are mandatory at this stage. To make our analysis more transparent, we consider a purely elastic matrix filled with periodically distributed plastic inclusions (see figure 4). We believe that will help the readers to get a better insight of the behavior and role of the elastic and plastic mechanisms.

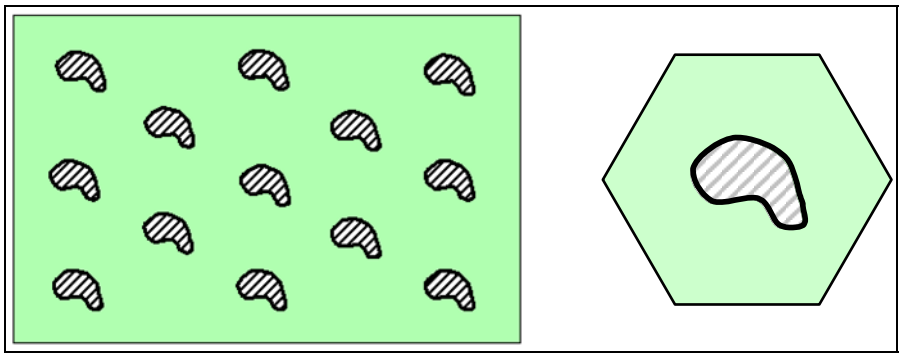

Figure 4. Elastic matrix with periodic distribution of "decks-of-cards."

The plastic inclusion possesses a single family of slip planes but it shows no elastic properties. This model of inclusion was coined as the "deck-of-cards" model. The matrix is assumed perfectly elastic, i.e., able to accumulate elastic energy. The inclusions behave like plastic solids: they are not able to accumulate any bulk elastic energy, instead they possess a single system of slip planes. Such a model appears to be simple enough to allow quite deep thermodynamic analysis.

When dealing with plastic deformations we ought to distinguish between the reference configuration R, the intermediate configuration I, and the actual configurations A (II). For deformable elasto-plastic inclusions and the "deck-of-cards" plasticity models, the configurations are shown in figure 5.

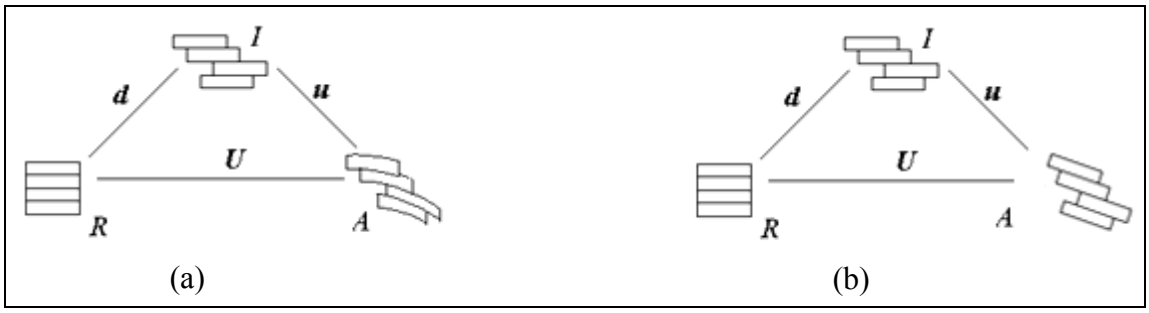

Figure 5. The configurations: (a) deformable inclusions and (b) "deck-of-cards" model.

Thus, we have to distinguish between the three boundary surfaces $S^R, S^I,$ and S^A of the same inclusion in the reference, intermediate, and actual configurations, respectively. Obviously, the surface S^I can be transformed into S^A by means of combined displacement and rotation.

3. The Kinematics and Energy of the "Deck-of-Cards" Model

Modern rigorous methods of homogenization begin with the analysis of the so-called "cell problem," which is a problem formulated for the elementary cell with periodic boundary condition. The elementary element for our problem is shown in figure 6. The simplest geometry and kinematics can be characterized by the two fixed-unit orthogonal vectors v^i and l^i, the scalar function of one variable $d(\rho)$, and the solid displacement D. In what follows, we call the unit vector l^i the sliding director. The solid displacement D includes the constant vector of translation a^i and a constant tensor of rotation $R^i_{.j}$.

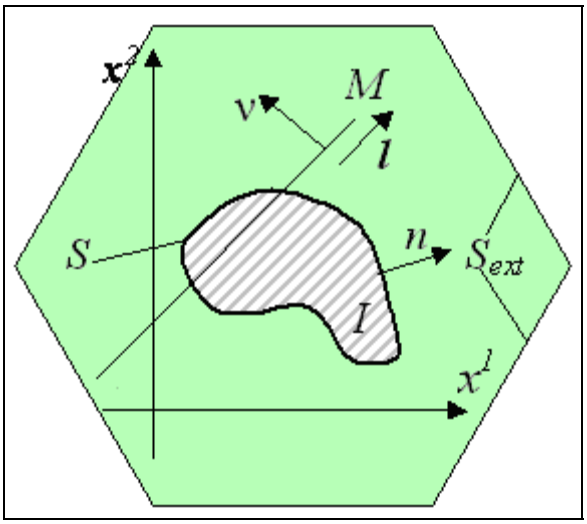

Figure 6. The geometry and kinematics of the elementary cell.

In the suggested model, the slip system consists of the one-parameter family of parallel planes with the unit normal **v** (in the reference and intermediate—but not actual—configurations). We postulate that all material points of the plane parallel to the basal plane at the distance h experience the same relative slip displacement $s^i = l^i d(h)$. The total displacement U^i of the point x^i of the inclusion can be decomposed into the distributed slip s and the displacement of the inclusion as rigid whole:

$$U^i(x) = a^i + R^i_{.k}\left(x^k + l^k d(h)\right) - x^i \ , \ h \equiv v_l x^l \ , \tag{1}$$

where a^i is the vector of translation, and $R^i_{.k}$ is the tensor of rotation.

The total displacements are assumed continuous displacements across the interface:

$$U^i\Big|_{inc} = u^i\Big|_{mat} , \tag{2}$$

where u^i is the displacement vector of the matrix.

We assumed that only matrix is capable of accumulating bulk energy. Let $\psi(u_{i|j})$ be the bulk energy density per unit volume of the matrix. The equation of equilibrium for the system can be established by applying the minimum energy principle to the energy functional

$$E = \int_{\omega} d\omega \, \psi(u_{i,j}) . \tag{3}$$

When minimizing the energy (equation 3), the continuity constraint (equation 2) should be taken into account.

With few exceptions, the elementary cell problem cannot be solved explicitly. There is one important case permitting further explicit analysis. It is the dilute concentration case, i.e., the case when the inclusions' dimensions are much smaller then the dimensions of the whole cell of periodicity. In the case of dilute concentration, instead of the problem with periodic boundary conditions one ought to consider a much simpler problem. This problem deals with a single inclusion within an unbounded domains subjected to specified displacement gradients at infinity:

$$u_i \to \Delta_{ij} x^j \ \ at \mid x^j \mid \to \infty . \tag{4}$$

In what follows, only this very problem will be analyzed.

4. The Exact System of Equilibrium Equations

The exact equations of equilibrium for this system can be derived by calculating the first energy variation of the total energy (equation 3) and separating the independent variation of the existing degrees of freedom. Not dwelling on the cumbersome details, we present the resulting system of equilibrium equations:

- the bulk equation of mechanical equilibrium within the bulk of the matrix

$$\frac{\partial}{\partial x^j}\frac{\partial \psi}{\partial u_{i|j}} = 0 ; \tag{5}$$

- the equation of zero resulting momentum acting on the inclusion

$$\int_S dS \frac{\partial \psi}{\partial u_{i|j}} n_j = 0 ; \tag{6}$$

- the equation of zero resulting moment of momentum

$$\varepsilon_{mkl} R_{i\cdot}^{\cdot l} \int_S dS \frac{\partial \psi}{\partial u_{i|j}} n_j \left(x^k + l^k d(v_p x^p) \right) = 0 ; \tag{7}$$

- and the equation for the slip distribution $d(h)$

$$\int_\Gamma d\Gamma \Theta(h,\gamma) \frac{\partial \psi}{\partial u_{i|j}} n_j R_{ik} l^k = 0 , \tag{8}$$

which should be satisfied for each contour Γ produced by intersection of the inclusions' interface S with each of the planes of the slip family. In equation 7, ε_{mkl} is the skew-symmetric tensor; in equation 8, Θ is a geometric factor characterizing the geometry of the interface S and of the slip system explained below.

The physical meaning of equations 5–8 is quite transparent. Equation 5 is a standard equation of equilibrium within the matrix. Equations 6 and 7 say that the resultant momentum and moment of momentum, acting on the deck-of-cards, should vanish. The integrand of the equation 8 gives the projection on the on the sliding director of the resulting force acting on each contour Γ. In this sense, equation 8 says that not only the inclusion as whole but each its slices should be in the state of full mechanical equilibrium under the action of the external forces acting from the deformable matrix on each slice.

5. The Geometric Factor

In order to define the factor $\Theta(h,\gamma)$, let us choose the special Gaussian coordinates (h,γ) on the inclusions' interface S^R. First of all, we parameterize the set of the parallel slip planes with the parameter ρ (see figure 7). For any two different planes with the coordinates h_1 and h_2, the difference $|h_2 - h_1|$ is just the distance between the planes (which is the same in all three configurations).

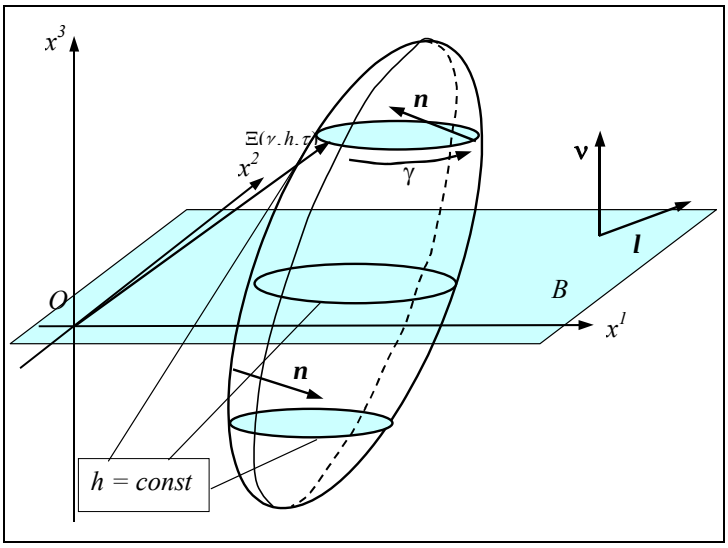

Figure 7. The geometric factor Θ.

For each h, we can introduce three different contours Γ_h^R, Γ_h^I, and Γ_h^A by intersecting the h-plane with the inclusion's surface in the reference, intermediate, and actual configurations. In the reference configuration, for each h we introduce the contour coordinates γ, obeying the following conditions: for each contour Γ_h^R the coordinate γ changes within the same interval I_γ, and the Gaussian coordinate system (h,γ) of the reference inclusions' boundary S^R is sufficiently smooth. The coordinates (h,γ) will be used as the materials coordinates of the particles belonging to the boundaries S^I and S^A in the intermediate and actual configurations.

In the intermediate configuration the line-element $d\Gamma_h^I(\gamma,h)$ of the contour Γ_h^I and the surface-element $dS^I(\gamma,h)$ of the surface S^I are given by the following formulas:

$$dS^I = \Xi^I(h,\gamma)dhd\gamma, \quad d\Gamma^I = G^I(\gamma,h)d\gamma. \tag{9}$$

Now, we can define the factor $\Theta(\gamma,h)$ as

$$\Theta(h,\gamma) \equiv \Xi^I(h,\gamma)/G^I(\gamma,h). \tag{10}$$

6. On the Quasi-Static Evolution

An inelastic slip along the slip planes is a relatively slow irreversible process as compared with two other time scales: with the time scale of establishing mechanical equilibrium within the matrix and with the time scale of establishing mechanical equilibrium of the inclusion as

whole. The inelastic sliding is opposed by the "plasticity" friction across the slip interfaces. In many situations, the equilibrium equation 8 should be replaced with the more realistic quasi-static equation

$$\pi(h,t) = -\mathrm{K}\int_{\Gamma} d\Gamma\Theta(h,\gamma)\frac{\partial\psi}{\partial u_{i|j}} n_j R_{ik} l^k, \quad \pi(h,t) \equiv \frac{\partial d(h,t)}{\partial t}, \tag{11}$$

where $\mathrm{K} > 0$ is a corresponding kinetic function, defining the rate of plastic slip and $\pi(h,t)$ is the slip velocity. The demand of thermodynamic consistency leads to the conclusion that the function K should be positive. However, it is not able to add anything more definite even about the arguments of this function. Based on the analogies with other kinetic problems, we should expect that the most important arguments of this function are the temperature of the system and the area of the slice.

In the quasi-static case, not only the slip-function $d = d(h,t),$ but all the unknown functions become the functions of time: $u^i = u^i(x,t)$, $a^i = a^i(t)$, $R^i_{\cdot j} = R^i_{\cdot j}(t)$. Their time evolution is characterized by the following relationships:

$$\frac{\partial u^i(x,t)}{\partial t} = V^i(x,t), \frac{da^i(t)}{dt} = A^i(t), \frac{dR^m_{\cdot k}(t)}{dt} = \varepsilon_{jkl}\Omega^j(t)R^{ml}_{\cdot\cdot}, \tag{12}$$

where $V^i(x,t)$ is the velocity of the matrix's particles, $A^i(t)$ is the translational velocity of the inclusion as whole, and the matrix's particles, $\Omega^j(t),$ are the angular velocity of the inclusion.

The relationships in equation 12 should be included in the master system of quasi-static evolution. This system should be also supplied with the initial conditions:

$$u^i(x,t) = a^i(t) = d(h,0) = 0,\ R^i_{\cdot j}(0) = \delta^i_j. \tag{13}$$

The condition (equation 4) at infinity should be replaced with the following:

$$V_i \to \kappa_{ij}x^j \ \ at\ |\ x^j\ | \to \infty. \tag{14}$$

7. How to Solve the Quasi-Static Master System Iteratively

It should be emphasized that the master system (equations 1, 2, 5–7, and 11–14) of quasi-static evolution is a deeply nonlinear one. It has several sources of nonlinearity. Among them are: the standard elastic nonlinearities (i.e., the nonlinearities associated with the elastic potential) and the specific nonlinearity, associated with the possibility of non-elastic slip. Formally, the latter source of nonlinearity is associated with the unknown function $d(h)$ which defines the inclusions' interface S geometry in the actual configuration.

Fortunately, this system can be solved iteratively, and each iteration is associated with solving a linear boundary value problem. The procedure is described as follows.

Assume that we already determined all the functions $u_i(x,t)$, $a(t)$, $R^i_{\cdot j}(t)$, and $d(h,t)$ up to a certain moment of time, $t = t_0$. Let us choose a sufficiently small time-step, Δt, and try to update these functions for the moment $t_1 = t_0 + \Delta t$. To that end, we first calculate the "velocity" functions $V_i(x,t_0)$, $A(t_0)$, $\Omega^j(t_0)$, and $\pi(h,t_0)$ by solving a linear boundary value problem. This linear boundary value problem includes the former of the relationships in equation 11. Other equations can be obtained by differentiating equations 1, 2, 4, 5–7, and 10 with respect to time. Then, we can update the functions $u_i(x,t)$, $a(t)$, $R^i_{\cdot j}(t)$, and $d(h,t)$, using the following relations:

$$\begin{aligned} &u_i(x,t_1) = u_i(x,t_0) + V_i(x,t_0)\Delta t,\ a(t_1) = a(t_0) + A_i(t_0)\Delta t, \\ &R^m_{\cdot k}(t_1) = R^m_{\cdot k}(t_0) + \varepsilon_{jkl}\Omega^j(t_0)R^{ml}_{\cdot\cdot}(t_0),\ d(h,t_1) = d(h,t_0) + \pi(h,t_0)\Delta t, \end{aligned} \tag{15}$$

inferred by equations 11 and 12. Then, we re-iterate the whole procedure.

8. A Spherical Deck-of-Cards Inclusion Within Isotropic Matrix

The initial velocities $V_i(x,t)$, $A(t)$, $\Omega^j(t)$, $\pi(h,t)$, and at $t = 0$ can be calculated explicitly for the instructive case of the initially spherical deck-of-cards within an isotropic matrix.

In the lowest order terms, the system (1, 2, 5–7, and 11) leads to the much simpler system:

- bulk equation of mechanical equilibrium

$$c^{ijkl}V_{k,lj} = 0; \tag{16}$$

- the kinematic constraint

$$V^i\big|_{S_0} = A^i + G^i_{\cdot k}\, x^k; \tag{17}$$

- the equation of zero resultant force acting on the inclusion

$$\int_{S_0} dS\, c^{ijkl}V_{k,l}n_j = 0; \tag{18}$$

- the equation of zero resultant moment of momentum acting on the inclusion

$$\varepsilon_{mki} c^{ijpq} \int_{S_0} dS V_{p,q} n_j x^k = 0 ; \tag{19}$$

- the kinetics equations

$$\frac{\partial \Pi(h,t)}{\partial t} = -\mathrm{K} c^{ijkl} \int_{\gamma_0} d\gamma \Gamma(h,\gamma) V_{k,l} n_j x^k l_i . \tag{20}$$

In the last system, we use the following notation S_0 for the inclusion in the initial configuration: $G^i_{\cdot j} \equiv \partial R^i_{\cdot j}(0)/\partial t$. At last, $c^{ijkl} = \partial^2 \psi(0)/\partial u_{i|j} \partial u_{k,l}$ is the tensor of the instantaneous elastic modules in the unstressed configuration.

In the case of an isotropic matrices, the elasticity tensor c^{ijkl} has the form

$$c^{ijkl} = \mu \left(\frac{2\nu}{1-2\nu} x^{ij} x^{kl} + x^{ik} x^{lj} + x^{il} x^{kj} \right), \tag{21}$$

where μ and ν are the shear modulus and the Poisson ratio, respectively.

The system (equations 16–21) with the condition (equation 14) at infinity allows the following solution:

$$\begin{aligned} & W_i = \kappa_{ij} x^j - 4(1-\nu) B_{ip} \left(\frac{1}{r} \right)_{,\ p} + B_{pq} \left(r + C \frac{1}{r} \right)_{,i}^{\cdot\cdot pq}, \ r \equiv \sqrt{\delta_{ij} x^i x^j} ; \\ & A^i = 0, \ G_{ij} = \frac{1}{2} \left(\kappa_{ij} - \kappa_{ji} \right), \end{aligned} \tag{22}$$

where the constant C and the tensor B_{pq} are equal to

$$C = \frac{1}{5} R^2 , \ B_{pq} = -\frac{5R^3}{4(4-5\nu)} \left(\frac{1}{5(1-2\nu)} \kappa^l_{\cdot l} x_{pq} + \kappa_{pq} \right), \tag{23}$$

and R is a radius of the inclusion.

At the matrix/inclusion interfaces the matrix's stresses $\sigma^{ij} n_j$ are equal to

$$\sigma^{ij} n_j = \mu \Gamma^i_{\cdot p} \frac{x^p}{r} \ , \tag{24}$$

with the tensor $\Gamma^{i}_{\cdot p}$ given by the formula

$$\Gamma^{i}_{\cdot p} \equiv \frac{1-\nu}{4-5\nu}\left(\kappa^{q}_{\cdot q}\delta^{i}_{p}\frac{11-10\nu}{1-2\nu}+15\kappa^{i}_{\cdot p}\right). \tag{25}$$

Inserting this relationship in equation 20, we arrive at the following formula for the rate of plastic slip at $t=0$:

$$\pi(h,0) = -\mathrm{K}\pi\frac{15(1-\nu)}{4-5\nu}\sqrt{R^2-h^2}\,\sigma^{12}. \tag{26}$$

Equation 26 shows that the quantity $\pi(h,0)/\mathrm{K}$ is the biggest at $h=0$, i.e., at the plane passing through the plane of the spherical deck-of-cards. It would be premature, however, to conclude that the rate of plastic slip is the biggest at this plane. In fact, the kinetic function K can depend upon the geometric characteristics of the cross-sections and completely suppress the role of the numerator π. Thermodynamics on its own has no means to do more than provide us with equation 26. The determination of the function K requires completely different methods, mostly experimental.

9. Conclusion

In this report, we discussed the problem of developing a thermodynamically consistent continuum theory of plasticity of ceramic-like materials, i.e., materials with limited plasticity. We assume that the substance is a polycrystal, i.e., a conglomerate of monocrystals. The limited plasticity is associated with limited number of slip planes of each monocrystal. Our ultimate goal is to derive macroscopic equations by averaging the aforementioned ensemble of monocrystals.

We made only the first step in the targeted direction by considering deformations and stresses within an isotropic infinite elastic matrix containing an inclusion. The inclusion is capable of relative slippage of its parts along a single family of parallel planes but is not capable of accumulated elastic energy. For this system, we established thermodynamically consistent conditions of equilibrium and quasi-static evolution. Also, we solved explicitly the simplest problem for the case of an initially spherical inclusion.

The results presented require further developments in several directions. Among them are the following:

- Accounting for the deformability of the “decks-of-cards,”
- Accounting for multiple independent slip systems,
- Development of full thermodynamic theory, including irreversible generation of heat,
- Further analysis of the simplest but instructive boundary value problems,
- Realization of the rigorous scheme of homogenizations and verification of the consistency of the Batdorf-Budyansky model, and
- Numerical implementation of suggested models.

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IMNE ALC IMS
2800 POWDER MILL RD
ADELPHI MD 20783-1197

1 DIRECTOR
US ARMY RESEARCH LAB
AMSRD ARL CI OK TL
2800 POWDER MILL RD
ADELPHI MD 20783-1197

1 DIRECTOR
US ARMY RESEARCH LAB
AMSRD ARL CI OK T
2800 POWDER MILL RD
ADELPHI MD 20783-1197

ABERDEEN PROVING GROUND

1 DIR USARL
AMSRD ARL CI OK TP (BLDG 4600)

NO. OF
COPIES ORGANIZATION

ABERDEEN PROVING GROUND

50 DIR USARL
AMSRD ARL CI HC
P CHUNG
AMSRD ARL SL
R COATES
AMSRD ARL WM
J MCCAULEY
T WRIGHT
AMSRD ARL WM MD
C FOUNTZOULAS
AMSRD ARL WM T
P BAKER
AMSRD ARL WM TA
C HOPPEL
C KRAUTHOUSER
B LEAVY
S SCHOENFELD
AMSRD ARL WM TB
S KUKUCK
AMSRD ARL WM TC
M FERMEN-COKER
R MUDD
B SCHUSTER
S SEGLETES
W WALTERS
AMSRD ARL WM TD
T BJERKE
S BILYK
D CASEM
J CLAYTON
T CLINE
D DANDEKAR
W EDMANSON
M GREENFIELD (20 CPS)
C GUNNARSON
Y HUANG
B LOVE
M RAFTENBERG
E RAPACKI
M SCHEIDLER
T WEERASOORIYA